Fermi Velocity Modulation in Graphene by Strain Engineering

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Abstract

Using full-potential density functional theory (DFT) calculations, we found a small asymmetry in the Fermi velocity of electrons and holes in graphene. These Fermi velocity values and their average were found to decrease with increasing in-plane homogeneous biaxial strain; the variation in Fermi velocity is quadratic in strain. The results, which can be verified by Landau level spectroscopy and quantum capacitance measurements of bi-axially strained graphene, promise potential applications in graphene based straintronics and flexible electronics.

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1 Introduction

Graphene, a single layer of carbon atoms arranged in a two-dimensional (2D) hexagonal lattice, displays remarkable mechanical and electronic properties promising many applications in nano-devices [1]. The novel properties of graphene arise from the linear energy dispersion near the K point of the hexagonal Brillouin zone (BZ):

$$E - E_F \approx \pm v_F \hbar k \tag{1}$$

where E_F is the Fermi energy, v_F is the Fermi velocity of electrons/holes near the K point of the BZ and $(\hbar k)$ is the momentum. Many graphene device characteristics depend on v_F. For instance, graphene's fine structure constant

$$\alpha_G = \frac{e^2}{4\pi\epsilon_0 \hbar v_F} \quad \text{(S. I. units)} \tag{2}$$

appears in the graphene device characteristics of graphene field effect transistor (GFET) [2]; for an ideal graphene with a uniform channel potential V_{ch}, the quantum capacitance of graphene is given by [3]:

$$C_G = \frac{2e^2 k_B T}{\pi(\hbar v_F)^2} \ln\left[2\left(1 + \cosh\frac{eV_{ch}}{k_B T}\right)\right] \tag{3}$$

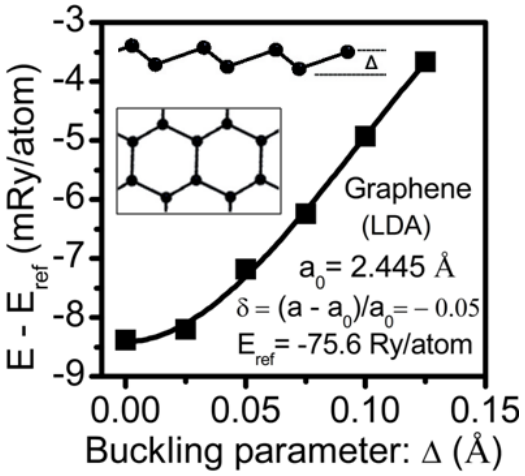
where T is the temperature and other symbols have their usual meanings. Thus, any change in v_F would affect the graphene device characteristics. Although strain-induced variation in v_F has recently been observed experimentally [4] by Raman spectroscopy study of uni-axially strained graphene, the quantitative dependence of v_F on strain remains unclear. Here, we report our theoretical investigation on the effect of biaxial strain on the Fermi velocity of charge carriers in graphene, which is experimentally known to sustain in-plane tensile elastic strain in excess of 20% [5]. Thus, our study mimics the experimental condition where graphene is supported on an ideal flat stretchable substrate.

2 Computational Methods

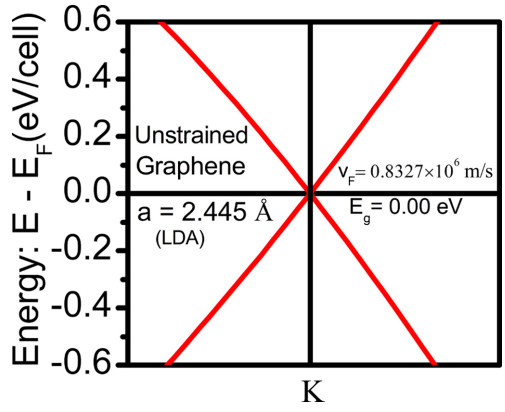
We use the DFT based full-potential (linearized) augmented plane-wave plus local orbital (FP-(L)APW+lo) method [6] as implemented in the elk code [7]. For the exchange-correlation term, we use the Perdew-Zunger variant of local density approximation (LDA) [8], the accuracy of which has been successfully tested in our previous works [9]. For plane wave expansion in the interstitial region, we have used $|\mathbf{G} + \mathbf{k}|_{max} \times R_{mt} = 9$, where R_{mt} is the muffintin radius, for deciding the plane wave cut-off. The k-point grid size of $30 \times 30 \times 1$ was used for all calculations. The total energy was converged within 2μ eV/atom. The 2D hexagonal structure of graphene was simulated by 3D hexagonal super cell construction with a large value of c-parameter ($|\mathbf{c}| = 40$ a.u.). The application of homogeneous in-plane biaxial δ strain was simulated by varying the in-plane lattice parameter $a(= |\mathbf{a}| = |\mathbf{b}|); \delta = (a - a_0)/a_0$, where a_0 is the ground state in-plane lattice constant.

3 Results and Discussions

In Figure 1(a), our calculated results show that under compressive strain of 5% graphene does not show any buckling, i.e. its planar structure remains preserved. Figure 1(b) depicts the linear energy band dispersion of unstrained graphene near the K point of the BZ. In Table 1, we compare our calculated values of a_0 and v_F with some reported values. Our calculated variation of Fermi velocity of electrons $v_F(e)$, holes $v_F(h)$



(a)



(b)

Figure 1: (a) Buckling probe of graphene at 5% compressive biaxial strain using the energy minimization procedure. Inset shows the side and the top-down views of buckled graphene in which alternate atoms in a hexagon reside on two different parallel planes; buckling parameter Δ is the perpendicular distance between these two planes; for planar graphene $\Delta = 0.00$Å. (b) Energy bands of unstrained graphene near K point of the BZ.

Table 1: Calculated values of a_0 and v_F compared with reported values.

a_0 (Å)	v_F (10^6 m/s)	Remark/Reference
2.4450	0.8327	This Work
2.4595	0.833	LAPW + GGA [10]
	0.79	Experiment, graphene on graphite substrate [11]
	1.093	Experiment, graphene on SiO_2/Si substrate [12]
	0.81	Experiment, single walled CNT [13]

and their average value $v_F = [v_F(e) + v_F(h)]/2$ at different strain values are shown in Figure 2. Since $v_F(h)$ values are slightly greater than $v_F(e)$ values, the band structure of electrons and holes are not exactly symmetric in qualitative agreement with a recent experiment [12] and the origin of this asymmetry is not well understood [12]. The decrease in Fermi velocity with increasing strain is due to a reduction in the π-orbital overlap [4]. Our calculated data in Figure 2 best fit with the following equations:

$$v_F(e) = 0.82386 - 1.26826 \times \delta + 0.71355 \times \delta^2 \quad (4)$$

$$v_F(h) = 0.84161 - 1.3269 \times \delta + 0.76501 \times \delta^2 \quad (5)$$

$$v_F = 0.83273 - 1.29758 \times \delta + 0.73928 \times \delta^2 \quad (6)$$

A possible precise measurement of the variation of v_F with δ may be carried out with Landau level spectroscopy study of a bi-axially strained graphene, since the Landau level spectrum is given by [12]:

$$E_n = E_D + \mathrm{sgn(n)} v_F \sqrt{2e\hbar B|n|} \quad (7)$$

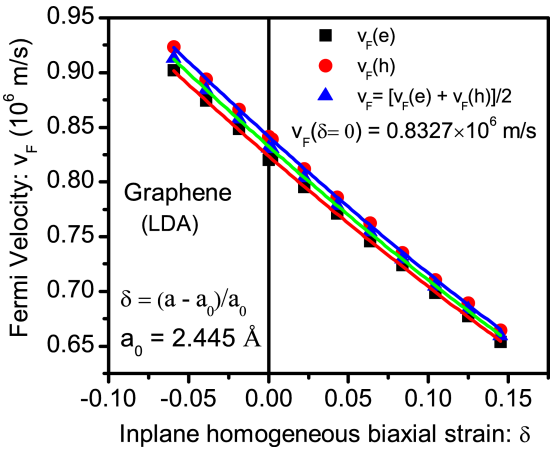


Figure 2: Fermi velocity variation with strain δ.

where n is an integer, E_D is the energy at the Dirac point, B is the magnetic field perpendicular to graphenes plane and other symbols have their usual meanings. Measurement of the quantum capacitance [3] of bi-axially strained graphene can also be useful.

4 Conclusions

There exists a small asymmetry in the Fermi velocity of electrons and holes in graphene whose reason is not yet clear. The Fermi velocity in graphene can be modulated by strain engineering for potential applications in graphene based flexible electronics.

References

[1] A. H. Castro Neto, et al., Rev. Mod. Phys. **81**, 109 (2009).

[2] F. Schwierz, Nature Nanotechnology **5**, 487 (2010).

[3] H. Xu, et al., Appl. Phys. Lett. **98**, 133122 (2011).

[4] M. Huang, et al., Nano Lett. **10**, 4074 (2010).

[5] C. Lee, et al., Science **321** (5887), 385 (2008).

[6] E. Sjöstedt, L. Nordström, D. J. Singh, Solid State Commun. **114**, 15 (2000).

[7] Freely available at: http://elk.sourceforge.net/

[8] P. Perdew, A. Zunger, Phys. Rev. B **23**, 5048 (1981).

[9] H. Behera , G. Mukhopadhyay, J. Phys. Chem. Solids **73**, 818 (2012); and other works cited in it.

[10] M. Gmitra, et al., Phys. Rev. B **80**, 235431 (2009).

[11] G. Li, et al., Phys. Rev. Lett. **102**, 176804 (2009).

[12] K.-C. Chuang, et al., Phil. Trans. R. Soc. A **366**, 237 (2008).

[13] W. Liang, et al., Nature **411**, 665 (2001).